

# NASA TECH BRIEF



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## Computer Program Determines Chemical Composition of Physical System at Equilibrium

### The problem:

In the course of study of any physical system in which chemical reactions play an important part, it is desirable to know the chemical composition of the system at thermodynamic equilibrium. The equilibrium chemical composition may indicate the maximum yields of the system obtainable under a given temperature and pressure, or it may reveal the maximum energy exchange possible. The classical approach to this problem is to examine the various chemical reactions involved and set up a group of nonlinear simultaneous equations based on the equilibrium constants, the temperature and pressure of the system, and the elemental mass balances. With even moderately complex systems, the resulting set of simultaneous equations is too difficult to solve to be practical.

### The solution:

A digital computer program written in FORTRAN IV for the IBM 7094 for the calculation of the equilibrium composition of complex, multiphase chemical systems.

### How it's done:

This program is based on the concept that at thermodynamic equilibrium the free energy of the system is at its minimum. Hence this method is known as the free energy minimization method. With this method, the equilibrium of each individual chemical reaction is not considered as such. Instead, attention is focused on the chemical potentials or the

free energies of the possible species. The distribution of these species is then established by minimizing the total free energy of the system. By this technique, the solution of the problem is reduced to mere mathematical operations, without concern for the chemistry involved.

The program is very general and may find applications in diversified areas. It is designed to cover a maximum of 12 elements in 80 gaseous and 15 condensed species. The elements included in the program are C, O, H, N, Si, A, Al, B, and Ca. The temperature range is 0 to 24,000 degrees K. Also certain thermodynamic properties of the system are determined as byproducts of the main calculations.

### Note:

Additional information is contained in North American Aviation, Inc. Report, "Digital Program Description for APD 104," SID 65-45, April 30, 1965, which is available from: COSMIC

Computer Center  
University of Georgia  
Athens, Georgia 30601  
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### Patent status:

No patent action is contemplated by NASA.

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